Molecular Simulation of Heat Shields

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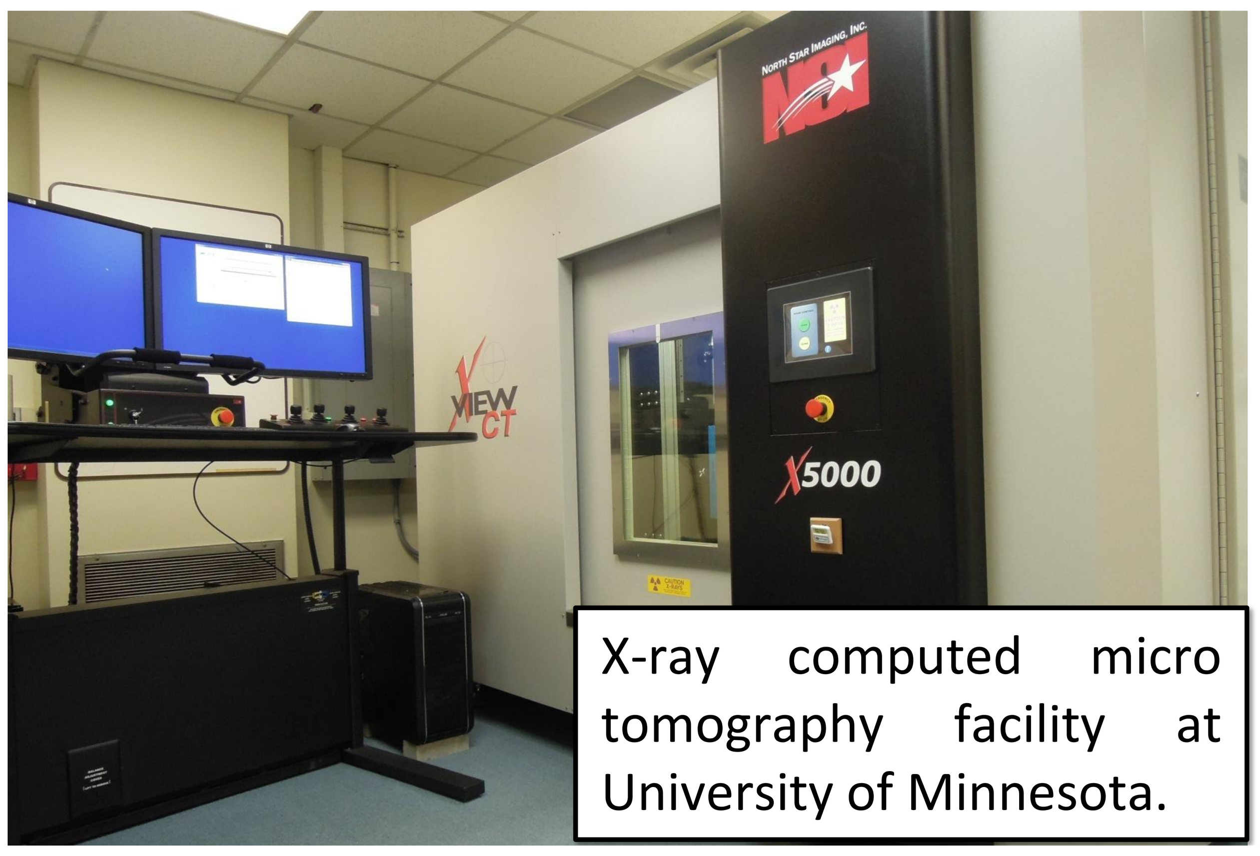
Molecular simulations are used to understand and model detailed physical processes occurring in both, porous and non-porous ablating heat shields. The microstructural surface of a real heat shield sample is obtained through 3D reconstruction using X-ray micro tomography and then used in the Direct Simulation Monte Carlo (DSMC) solver Molecular Gas Dynamics Simulator [1] to perform molecular simulations.

The goal of such molecular modeling is to understand ablation physics at the most fundamental level, in order to reduce uncertainty margins on heat shield and to design better thermal protection systems for future hypersonic missions.

X-ray computed tomography and surface grid for simulations

X-ray computed tomography (X-ray CT) is used to generate a 3D image of the inside of the object from a large series of two-dimensional radiographic images taken around a single axis of rotation [2].



X-ray computed micro tomography facility at University of Minnesota.

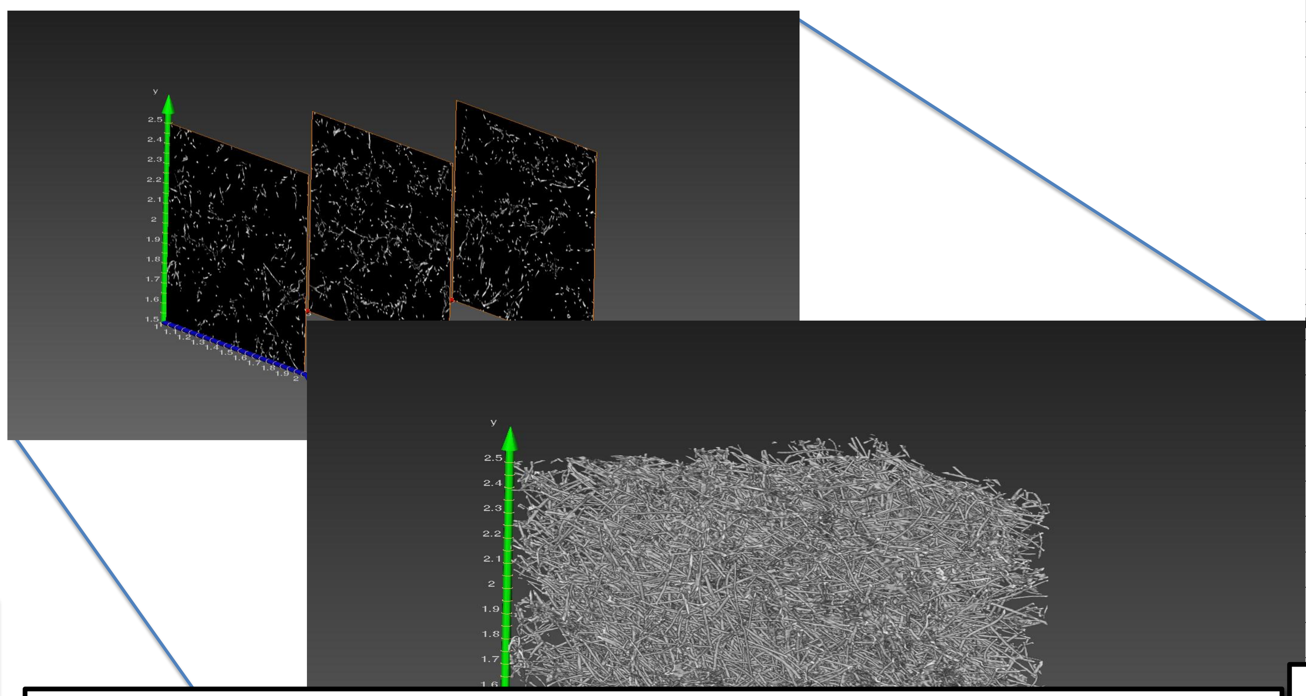
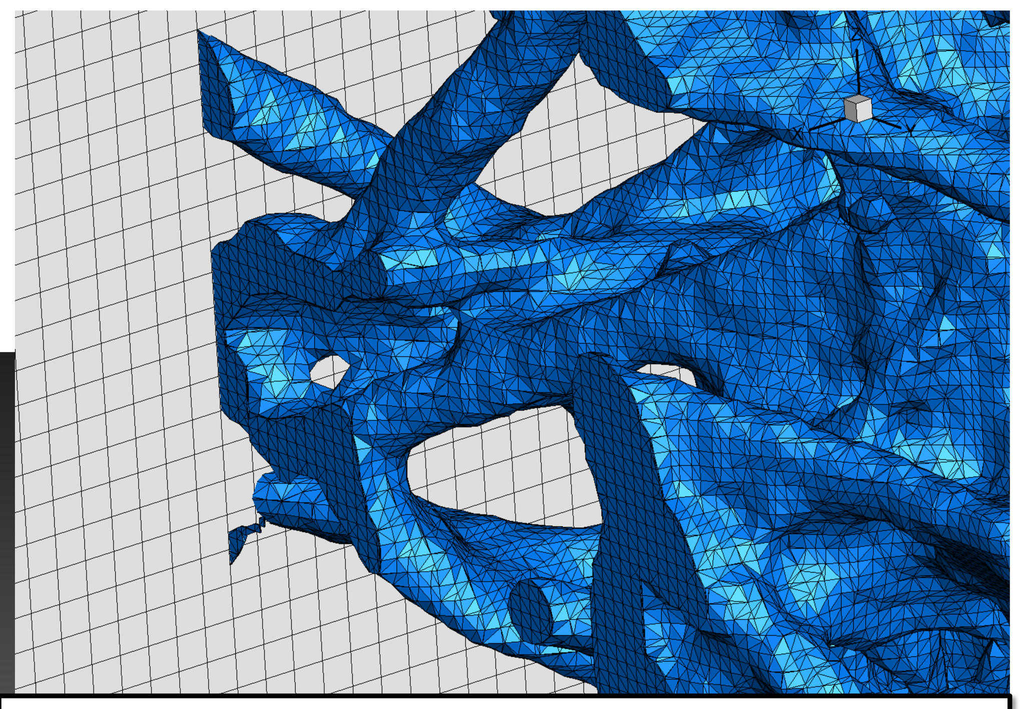
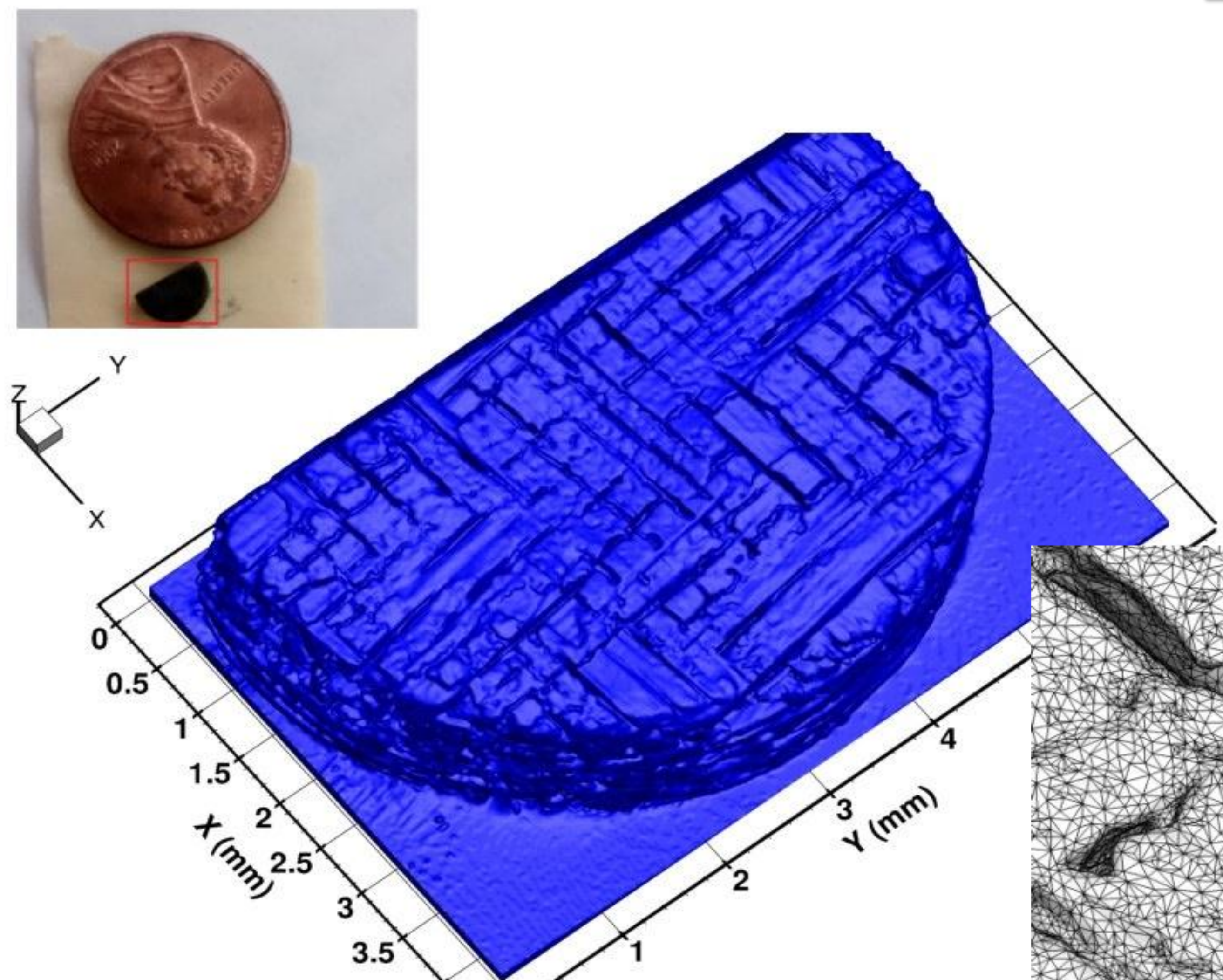


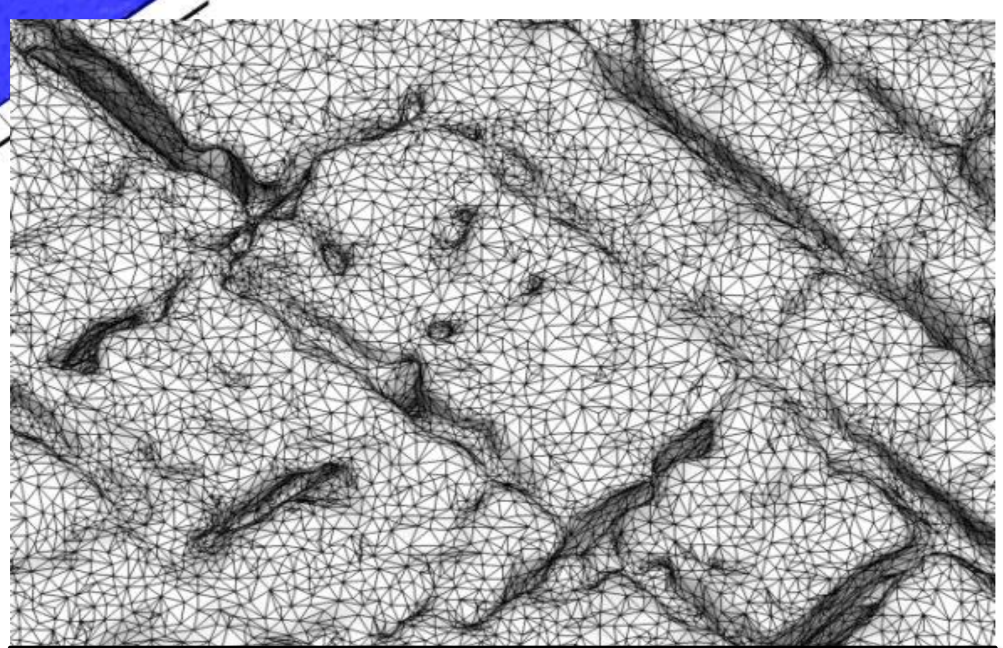
Illustration of the reconstruction of a 3D surface from the 2D slices from tomography.



Demonstration of the robust cut-cell algorithm [3] applied to a porous microstructure obtained from microtomography.



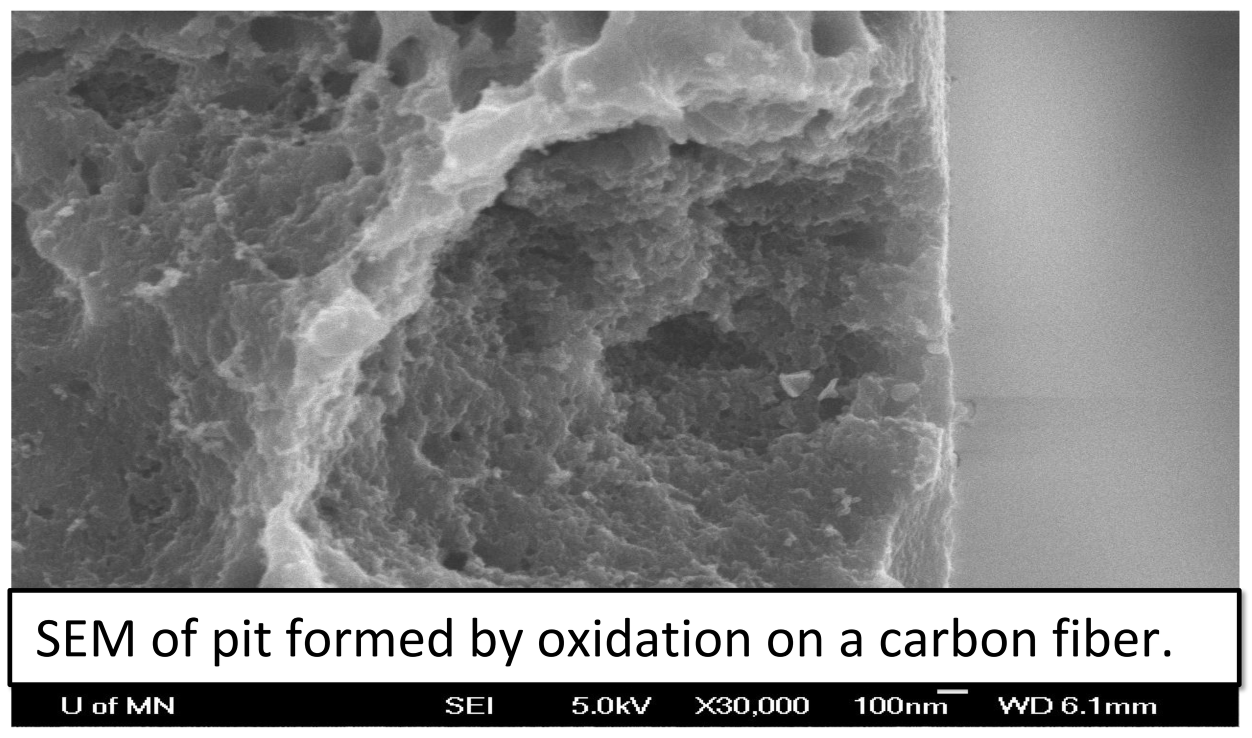
3D reconstructed surface of a Carbon-Carbon composite. The sample is shown in the inset.



Surface grid of 5 million triangles[3] on a real C-C composite.

Atomistic analysis of carbon based heat shields

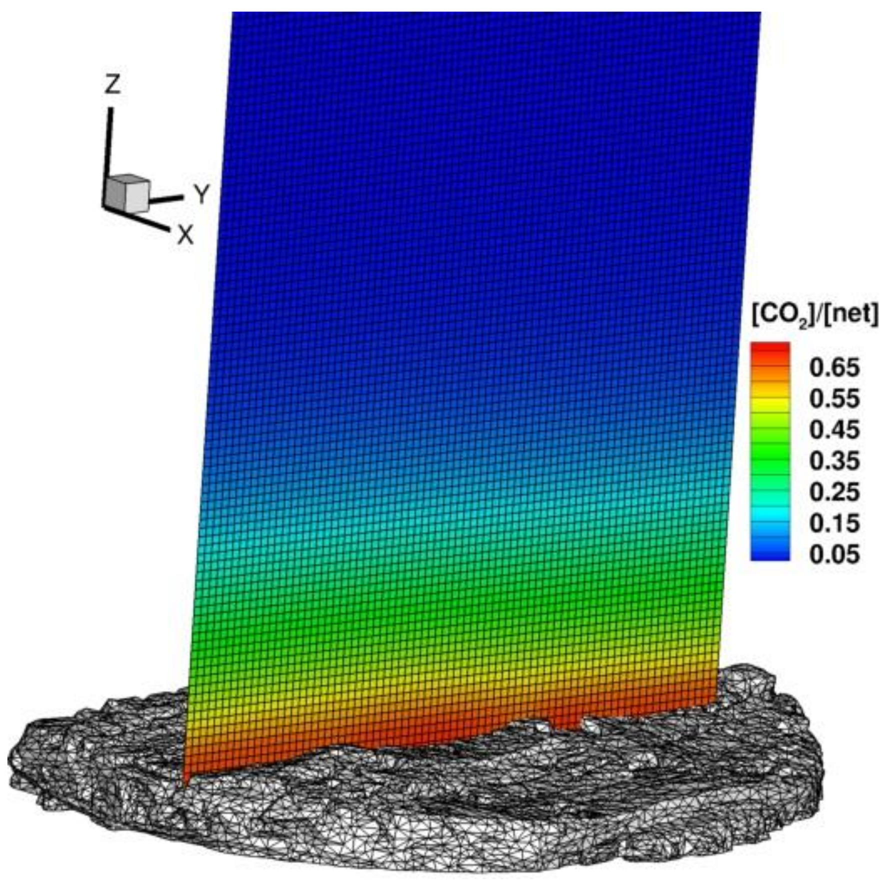
Atomistic analysis provides detailed data on the chemical reactions occurring on a carbon surface. The analysis is aided through experiments [4] and SEM images. The molecular beam data is used as input for DSMC boundary conditions to propose oxidation model for full vehicle CFD simulations.

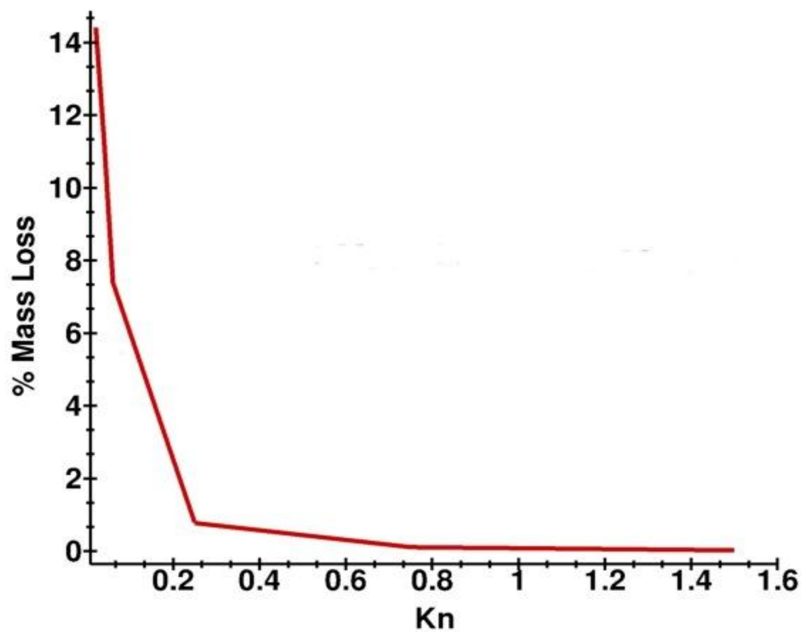


SEM of pit formed by oxidation on a carbon fiber.

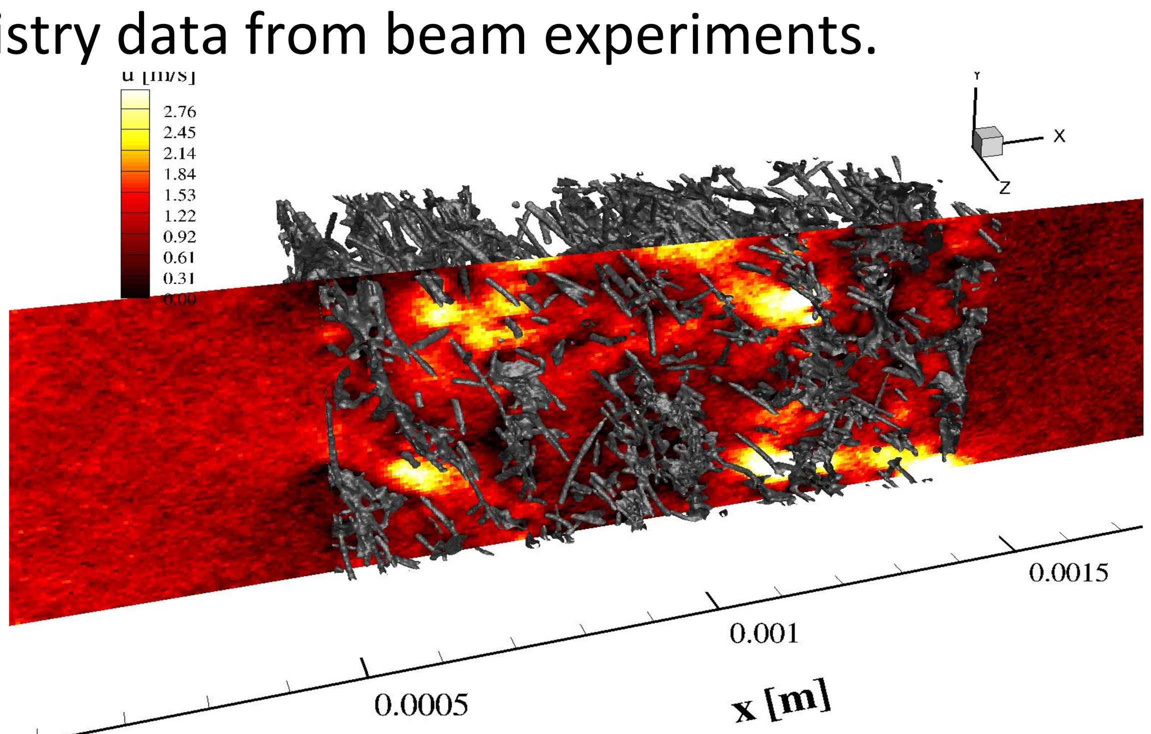
Flow study at the micro scale using DSMC

DSMC simulations are performed using the real surface and reaction chemistry data from beam experiments.





DSMC simulations of flow over the real C-C composite. CO_2 production is observed due to gas phase reactions [5] within the gaps of the fibers despite CO being the dominant product at the atomistic scale. Higher mass loss is observed due to such gas-phase reactions.



U-velocity contours from a DSMC Simulation of pressure driven flow through FiberForm. Surface generated using data from micro-tomography contains over 6 million triangular surface elements.

References

1)Nompelis I., Schwartzentruber T.E., AIAA 2013-1204.
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3)Zhang C., Schwartzentruber T.E., Computers and Fluids, Vol. 69, 2012.
4)Murray et. al., J. Phys. Chem C., Web Publication Mar 26 2015.
5)Poovathingal et. al., AIAA 2015-1449.

Acknowledgments

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